The University of Nottingham

Automated probe microscopy via evolutionary optimization at the atomic scale

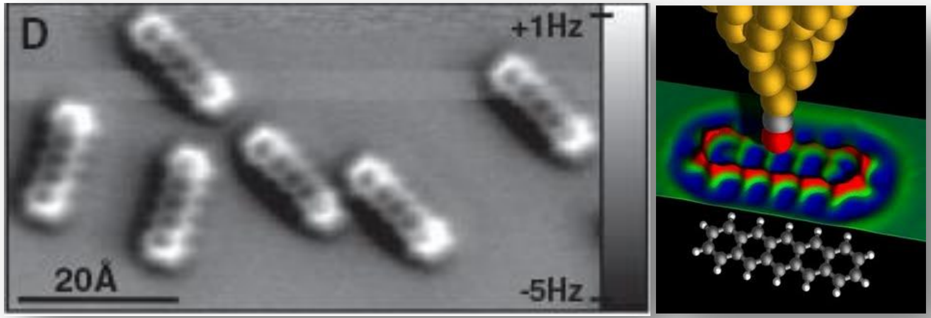
9^{th} Annual HUMIES Awards

Richard Woolley

richard.woolley@nottingham.ac.uk

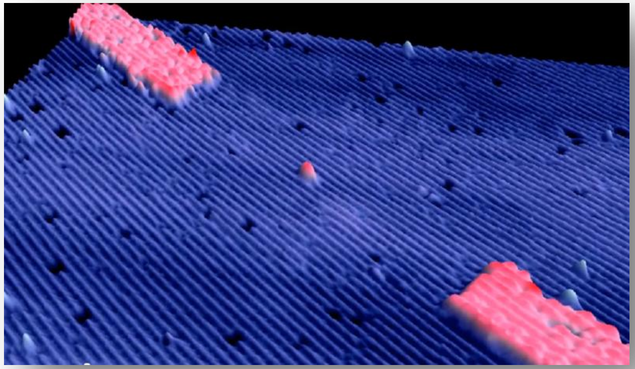
Julian Stirling, Adrian Radocea, Prof. Philip Moriarty, Prof. Natalio Krasnogor

The Power of Scanning Probe Microscopy



Imaging individual molecules and resolving sub molecular structure

Gross *et al.* Science 325, 1110 (2009)

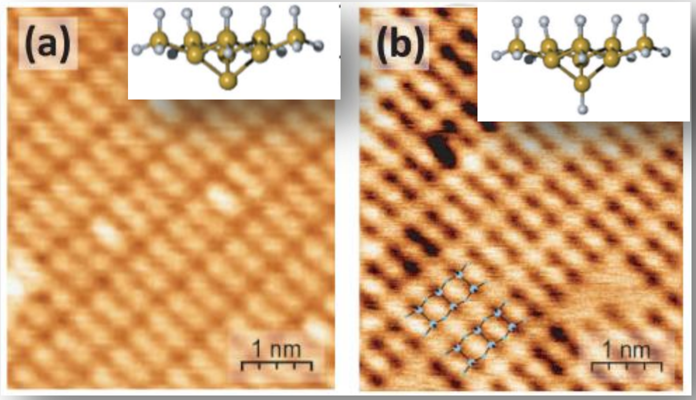


The ability to fabricate electronic devices (a single atom transistor) with atomic precision.

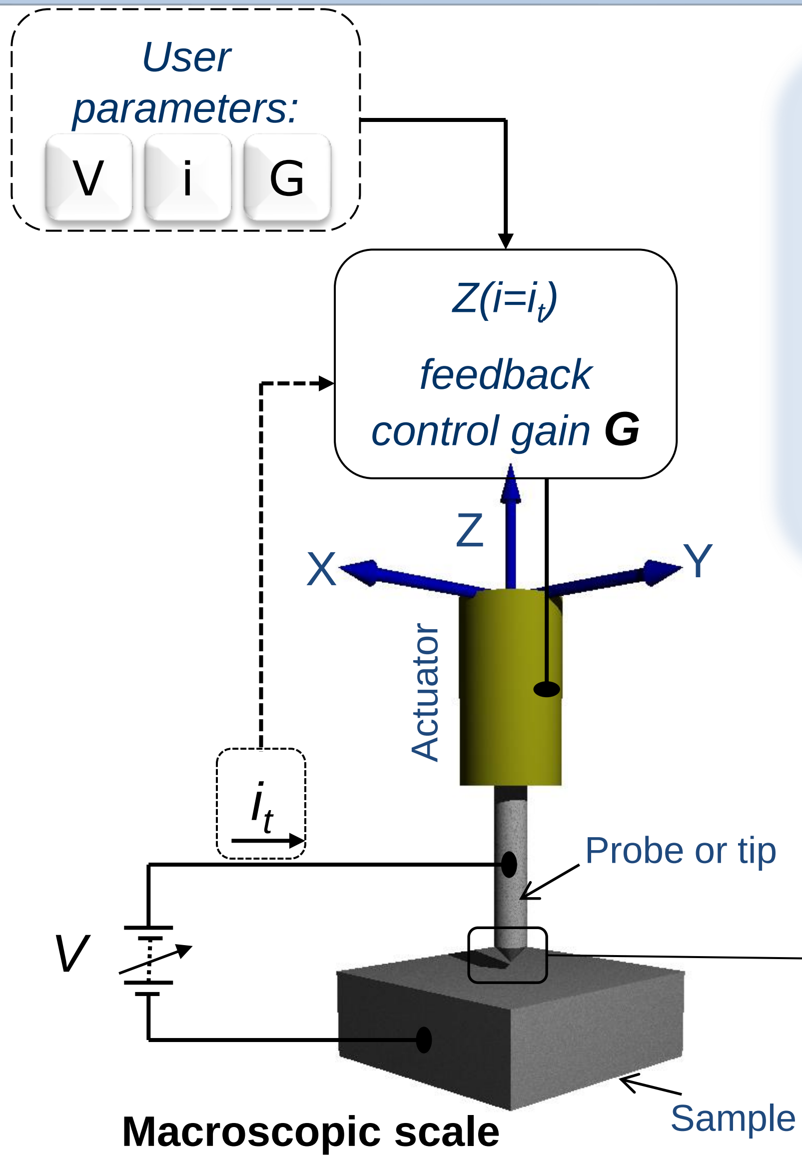
Fuechsle *et al.* Nature Nanotechnology 7, 242–246 (2012)

The importance of the probe structure; a single H atom at the probe apex inverts the image contrast.

Sharp *et al.* Appl. Phys. Lett. 100, 233120 (2012)



Scanning Tunneling Microscopy



Imaging parameters:

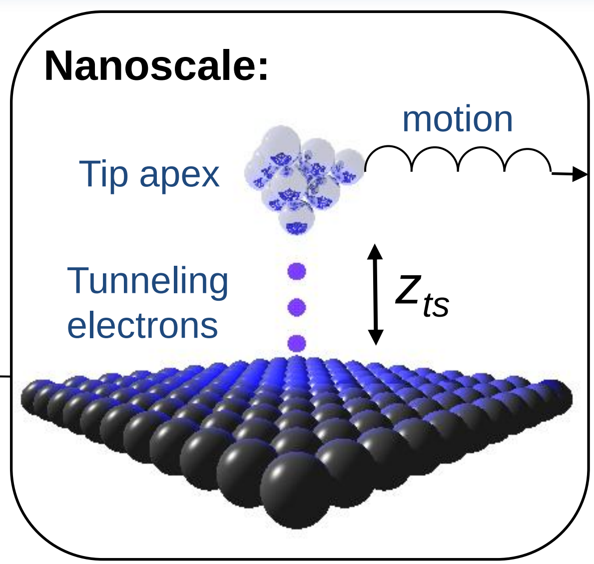
Tunnel current, i_t

Voltage, V

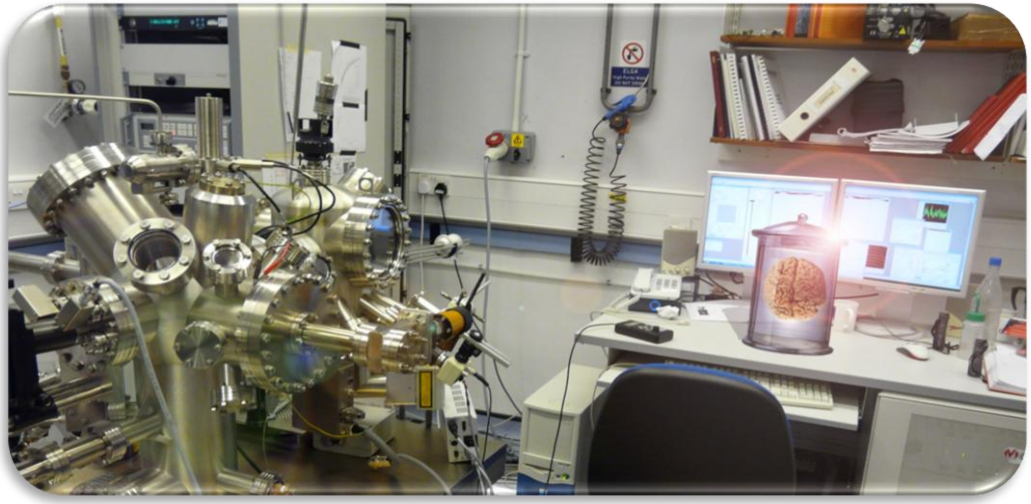
Gain, G

$$i_t \propto V\exp(-2kz_{ts})$$

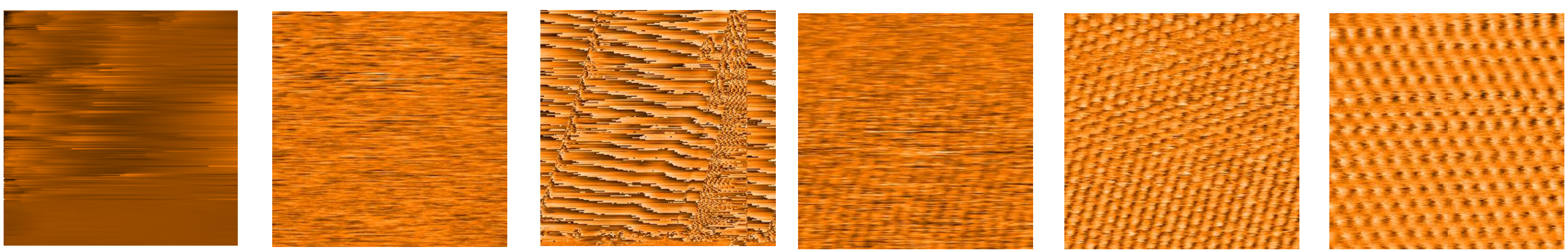
Where the tip-sample separation, z_{ts}, is maintained by a feedback loop of gain, G.



30 years without a solution, until now
(Criteria E & G)



- Thousands of users world wide
- Expensive machine and operator costs
- Many hours spent manually optimising images

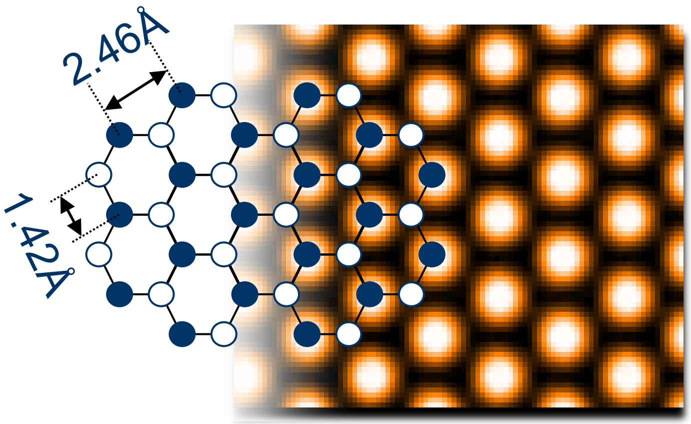


The problems:

•Changing tip state and,

•Obtaining the optimum imaging parameters ***V, i*** and ***G***

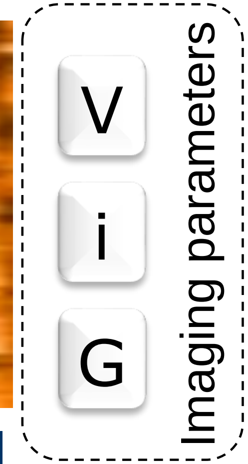
Fitness and the cGA



Target Image, T

Fitness=RMI(T,I)

Acquired Image, I



The cGA:

An individual, n, with imaging parameters V_n, i_n and G_n

The population of N individuals, each with imaging parameters V, i, G

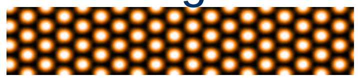
E.Alba and B. Dorronsoro, Cellular Genetic Algorithms (Springer 2008) ; Q.H. Quang et al., Evol. Comp. 17 231 (2009)

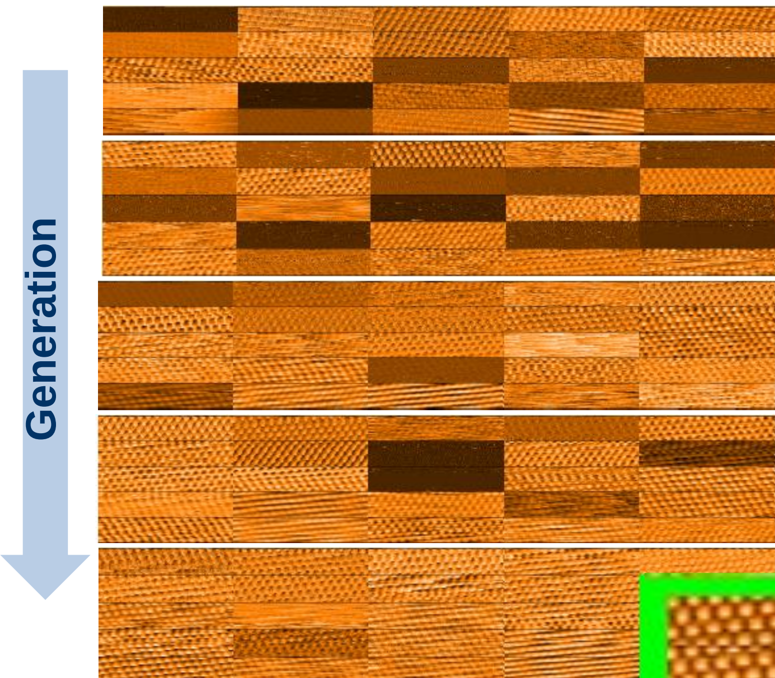
The cGA in operation

(Criteria F)

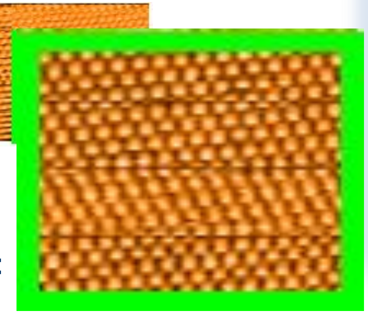
Start

Target



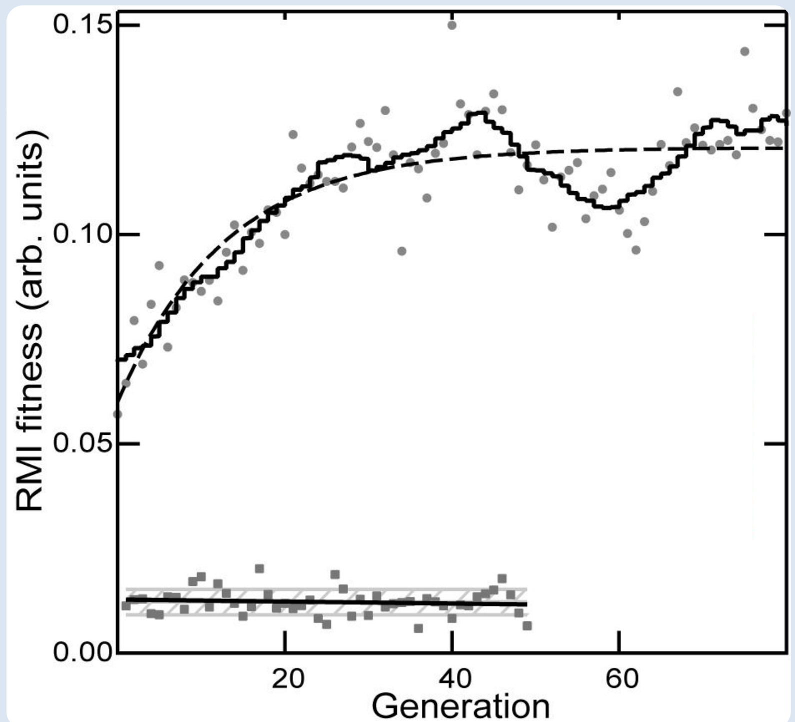


Final=



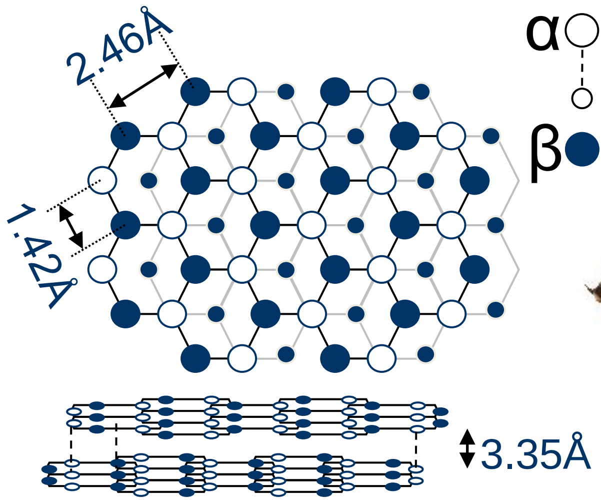
- Images taken by microscope for the individual’s parameters V, i, G
- Migrate good V, i, G

Generation vs. Fitness

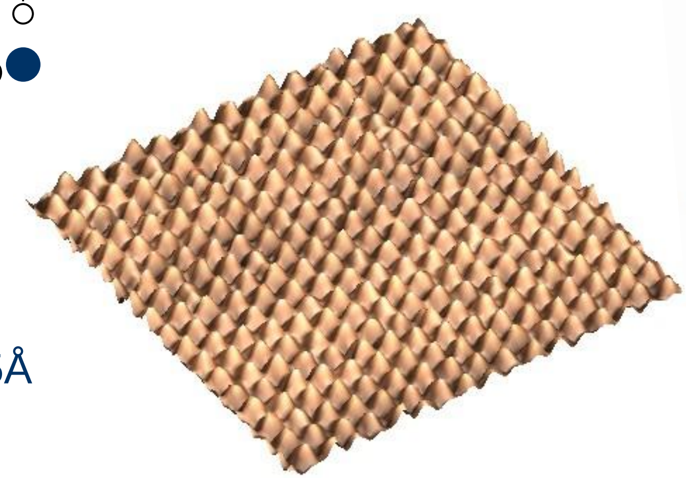


Can we choose different tip states?

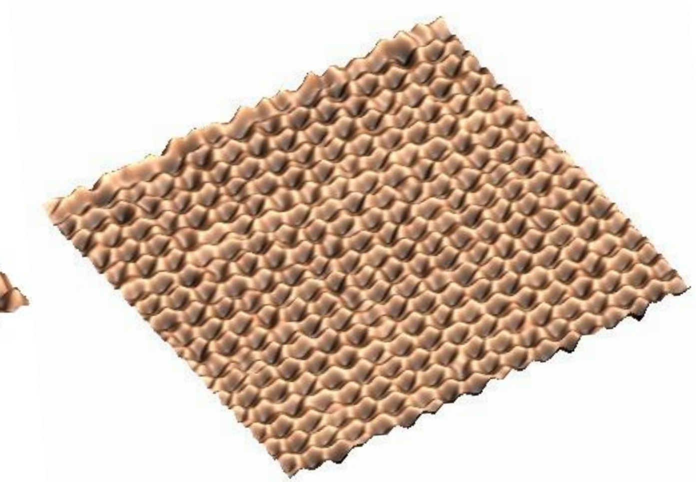
(Criteria E & D)



Triangular

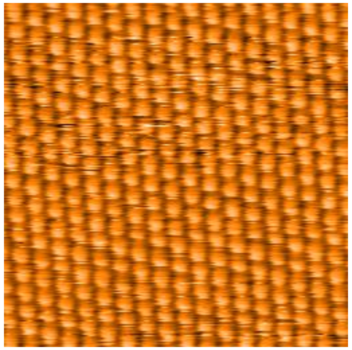


Honeycomb

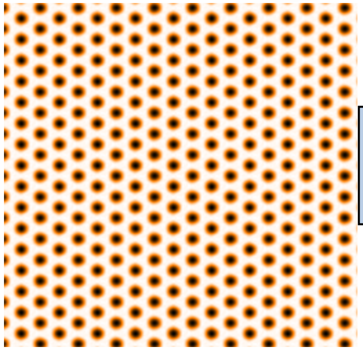


Triangular target

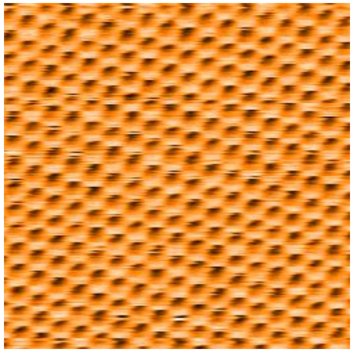
Triangular image



Honeycomb target



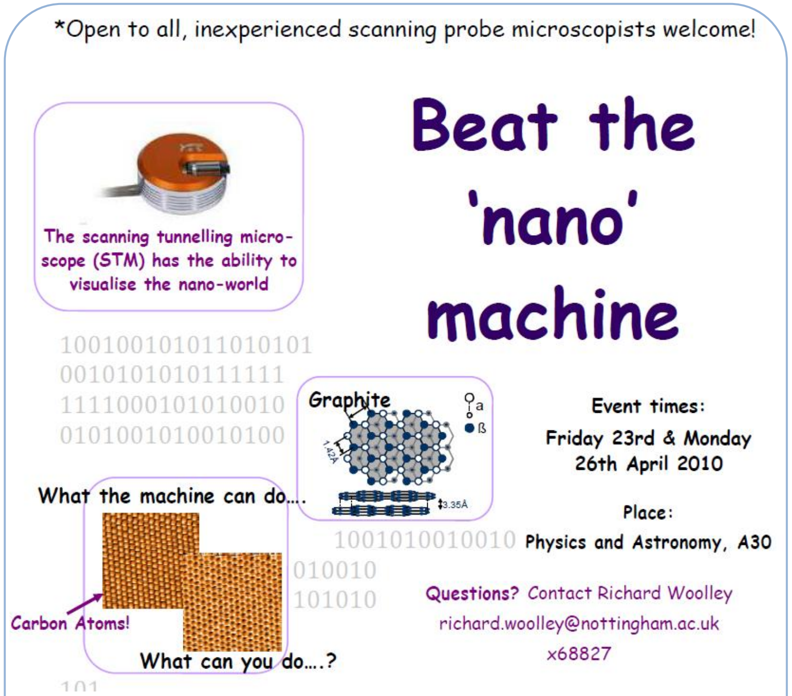
Honeycomb image



R.A.J. Woolley, J.Stirling, A. Radocea, N. Krasnogor, and P.J. Moriarty, Appl. Phys. Lett. 98, 253104 (2011)

Is it comparable to the human operator?

(Criteria H)



The Competition (Human vs. Machine):

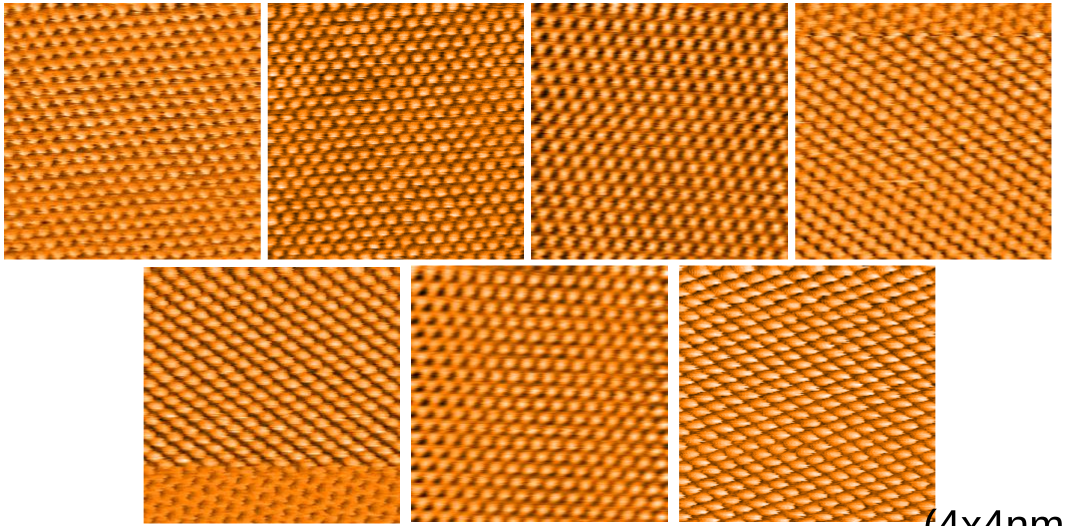
Obtain the best image possible within 1 hour

Results of the challenge

Microscopist	Average image quality	Change in image quality per min
Machine	0.20*	7.1*
Human	0.09	2.6

*winner

A selection of the machine optimised images:



($4x4nm^2$)

Criteria for human-competitiveness

(A) The result was patented as an invention in the past, is an improvement over a patented invention, or would qualify today as a patentable new invention

- New invention
- Working with the leading manufacturer

(D) The result is publishable in its own right as a new scientific result independent of the fact in was mechanically created.

- R.A.J. Woolley, J.Stirling, A. Radocea, N. Krasnogor, and P.J. Moriarty, Appl. Phys. Lett. 98, 253104 (2011)
- The same journal as the original Nobel prize wining invention

(E) result >= the most recent human-created solution to a long-standing problem for which there has been a succession of increasingly better human-created solutions.

- The human operator was the solution

Criteria for human-competitiveness

(F) result >= a result that was considered an achievement in its field at the time it was first discovered.

- The system is state of the art

(G) The result solves a problem of indisputable difficulty in its field.

- “That’s impossible”
- “Can we have it, please?”

(H) The result holds its own or wins a regulated competition involving human contestants (in the form of either live human players or human-written computer programs)

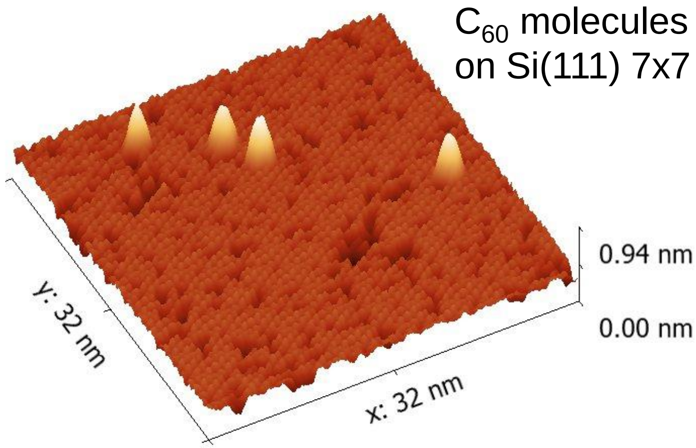
- The ‘Nano-machine’ won!

Summarising why this entry is best!

- *A step-wise change in STM operation for over 30 years*
- *An underpinning technology for the wider scanning probe instrumentation sector*
- *Innovative*
- *Greatly improved productivity*
- *State of the art*
- *Meets 6 out of the 8 criterion*

- *It's just the tip of the iceberg….*

Potential Future Impact



What does the future hold for a robot that can recognise atoms and molecules…

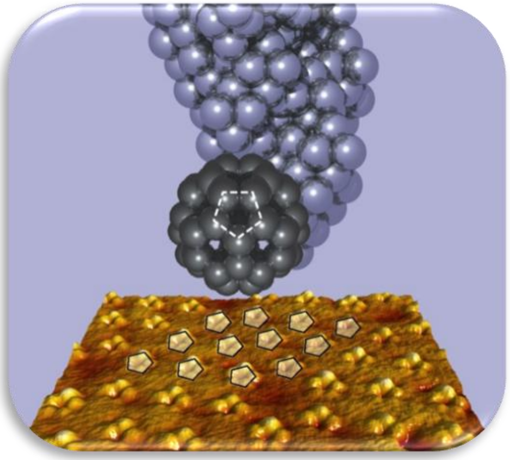


Image courtesy of S. Jarvis

….and can develop the nanoscale tools and necessary protocols to manipulate those atoms and molecules?

What would you get the robot to build?

*What if it evolved things that **it** wanted to?*

Thanks

Julian Stirling and
Prof. Philip Moriarty

School of Physics and Astronomy, The University of Nottingham, University Park, Nottingham, England

Prof. Natalio Krasnogor

Computer Science, The University of Nottingham, Jubilee Campus, Nottingham, England

Adrian Radocea

Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

EPSRC
Engineering and Physical Sciences Research Council

The authors would like to thank the EPSRC (Grant no: EP/H010432/1) and the European Commission's ICT-FET programme via the *Atomic Scale and Single Molecule Logic gate Technologies* (AtMol) project, Contract No. 270028 for providing financial support to this project.

richard.woolley@nottingham.ac.uk

www.nottingham.ac.uk/physics/research/nano

http://icos.cs.nott.ac.uk/